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NEWS 5	APR 28	IMSRESEARCH reloaded with enhancements
NEWS 6	MAY 30	INPAFAMDB now available on STN for patent family searching
NEWS 7	MAY 30	DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS 8	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS 9	JUN 06	KOREAPAT updated with 41,000 documents
NEWS 10	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS 11	JUN 19	CAS REGISTRY includes selected substances from web-based collections
NEWS 12	JUN 25	CA/CAplus and USPAT databases updated with IPC reclassification data
NEWS 13	JUN 30	AEROSPACE enhanced with more than 1 million U.S. patent records
NEWS 14	JUN 30	EMBASE, EMBAL, and LEMBASE updated with additional options to display authors and affiliated organizations
NEWS 15	JUN 30	STN on the Web enhanced with new STN AnaVist Assistant and BLAST plug-in
NEWS 16	JUN 30	STN AnaVist enhanced with database content from EPFULL
NEWS 17	JUL 28	CA/CAplus patent coverage enhanced
NEWS 18	JUL 28	EPFULL enhanced with additional legal status information from the epoline Register
NEWS 19	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS 20	JUL 28	STN Viewer performance improved
NEWS 21	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced
NEWS 22	AUG 13	CA/CAplus enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS 23	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS 24	AUG 15	CAplus currency for Korean patents enhanced
NEWS 25	AUG 25	CA/CAplus, CASREACT, and IFI and USPAT databases enhanced for more flexible patent number searching
NEWS 26	AUG 27	CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information
NEWS 27	SEP 18	Support for STN Express, Versions 6.01 and earlier, to be discontinued

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 NEWS 28  SEP 25  CA/CAplus current-awareness alert options enhanced
                  to accommodate supplemental CAS indexing of
                  exemplified prophetic substances
 NEWS 29  SEP 26  WPIDS, WPINDEX, and WPIX coverage of Chinese and
                  and Korean patents enhanced
 NEWS 30  SEP 29  IFICLS enhanced with new super search field
 NEWS 31  SEP 29  EMBASE and EMBAL enhanced with new search and
                  display fields
 NEWS 32  SEP 30  CAS patent coverage enhanced to include exemplified
                  prophetic substances identified in new Japanese-
                  language patents

 NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
              AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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=> file reg
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                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

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DICTIONARY FILE UPDATES:  29 SEP 2008  HIGHEST RN 1055027-88-7

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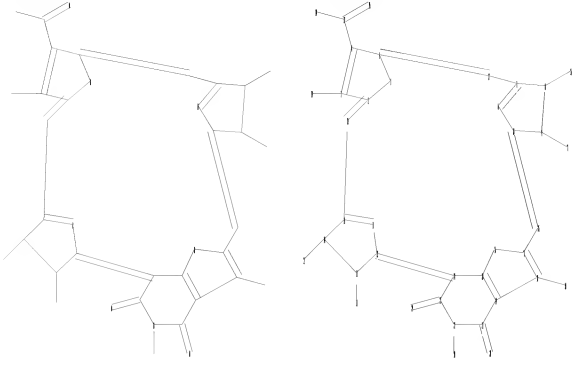

chain nodes :
28 29 30 31 32 33 34 35 36 37 38 39
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27
chain bonds :
3-39 4-33 8-36 9-37 13-31 14-32 18-38 21-28 22-30 23-29 33-34 33-35
ring bonds :
1-2 1-5 2-3 2-25 3-4 4-5 5-27 6-7 6-10 7-8 7-27 8-9 9-10 10-26 11-12
11-15 12-13 12-24 13-14 14-15 15-25 16-17 16-20 17-18 17-26 18-19 19-20
19-21 20-24
21-22 22-23 23-24
exact/norm bonds :
1-2 1-5 7-8 8-9 9-10 12-13 13-14 14-15 16-17 16-20 19-21 21-22 21-28
22-23 22-30 23-24 23-29 33-35
exact bonds :
3-39 4-33 8-36 9-37 13-31 14-32 18-38 33-34
normalized bonds :
2-3 2-25 3-4 4-5 5-27 6-7 6-10 7-27 10-26 11-12 11-15 12-24 15-25 17-18
17-26 18-19 19-20 20-24

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS 30:CLASS
31:CLASS 32:CLASS
33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS

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L1      STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1              STR

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Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 09:53:13 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       11 TO ITERATE

100.0% PROCESSED       11 ITERATIONS                                 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:           22 TO      418
PROJECTED ANSWERS:               2 TO      124

L2            2 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 09:53:17 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      193 TO ITERATE

100.0% PROCESSED      193 ITERATIONS                                29 ANSWERS
SEARCH TIME: 00.00.01

L3           29 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   178.36     178.57

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FILE COVERS 1907 - 1 Oct 2008 VOL 149 ISS 14
FILE LAST UPDATED: 30 Sep 2008 (20080930/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

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=> s l3
L4 20 L3

=> d l4 1-20 ibib abs hitstr

L4 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:975114 CAPLUS <<LOGINID::20081001>>
DOCUMENT NUMBER: 149:274976
TITLE: Activatable photodynamic therapy agents, conjugates comprising substrate, attached to photoactivatable killing agent, and quencher
INVENTOR(S): Zheng, Gang; Glickson, Jerry D.; Chance, Britton; Delikatny, Edward James; Stefflova, Klara; Chen, Juan
PATENT ASSIGNEE(S): University of Pennsylvania, USA
SOURCE: U.S. Pat. Appl. Publ., 68pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20080193431	A1	20080814	US 2006-383487	20060515
WO 2005048944	A2	20050602	WO 2004-US38024	20041115
WO 2005048944	A3	20060504		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:
US 2003-519794P P 20031114
US 2004-558501P P 20040401
WO 2004-US38024 A2 20041115
US 2005-695156P P 20050629

AB The present invention relates to the field of conjugates comprising a substrate which is attached to at least one photoactivatable killing agent and at least one first quencher, and methods for their use. More particularly, the present invention relates to photodynamic therapy agents. The invention further relates to methods for decontaminating blood and methods for treating cancer or viral infection in a subject using the conjugates of the present invention. Thus, conjugate with

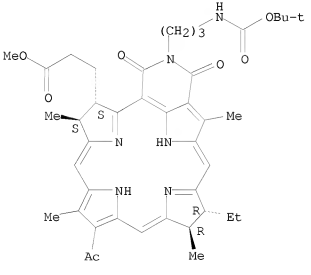
phospholipid as substrate was prepared: PLA2-specific phospholipid probe was synthesized incorporating both the quencher [e.g., carotenoid (Car)] and the PDT agent (e.g., Pyro) into the sn-1 and sn-2 portion of the phospholipid, resp.; this design makes the release of the fluorescent moiety independent of cleavage by phospholipase C and phospholipase D; furthermore, in order to have the phospholipase A2 specificity, the quencher is introduced into the sn-1 position via an ether linkage, since the ether linkage is resistant to phospholipase A1. Thus, O-alkylation of sn-glycero-3-phosphocholine with N-Boc-ethylene bromide in the presence of a cesium catalyst gives a mixture of mono sn-1, mono sn-2 and bis-conjugate, which is separated by HPLC; the sn-2 resulting intermediate will be coupled to the Pyro; after treating with trifluoroacetic acid to remove the Boc protection group, the amino group at the sn-1 position is conjugated to the quencher; the resulting phospholipid, thus, is PLA2-specific.

IT 810676-08-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(activatable photodynamic therapy agents)

RN 810676-08-5 CAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-19-[3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

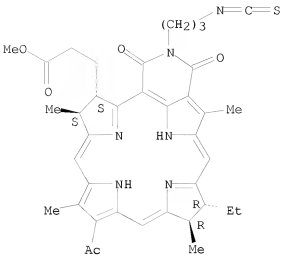


IT 810676-12-1P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(activatable photodynamic therapy agents)

RN 810676-12-1 CAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-1,5,6,15,16,18,19,20-octahydro-19-(3-isothiocyanatopropyl)-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:253145 CAPLUS <<LOGINID::20081001>>
DOCUMENT NUMBER: 148:302470
TITLE: Conjugates of RDG peptides and porphyrin or (bacterio)chlorophyll photosensitizer and their uses
INVENTOR(S): Scherz, Avigdor; Salomon, Yoram; Rubinstein, Efrat; Brandis, Alexander; Eren, Doron; Neimann, Karin
PATENT ASSIGNEE(S): Yeda Research and Development Co. Ltd., Israel
SOURCE: PCT Int. Appl., 191pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008023378	A1	20080228	WO 2007-IL1055	20070823
WO 2008023378	A9	20080410		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			
US 20080138278	A1	20080612	US 2007-843996	20070823

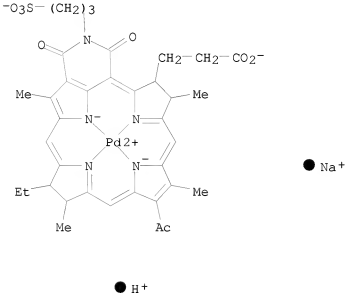
PRIORITY APPLN. INFO.: US 2006-839409P P 20060823
OTHER SOURCE(S): MARPAT 148:302470
AB Conjugates of porphyrin, chlorophyll and bacteriochlorophyll photosensitizers with RGD-containing peptides or RGD peptidomimetics are provided that are useful for photodynamic therapy (PDT), particularly vascular-targeted PDT (VTP), of tumors and nonneoplastic vascular diseases

such as age-related macular degeneration, and for diagnosis of tumors by different techniques.

IT 1010076-91-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(conjugates of RDG peptides and porphyrin or (bacterio)chlorophyll photosensitizer and their uses)

RN 1010076-91-1 CAPLUS

CN Palladate(2-), [(5R,6R,15S,16S)-10-acetyl-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-19-(3-sulfopropyl)-9,12-imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoato(4-)-κN1,κN23,κN24,κN25]-, sodium hydrogen (1:1:1), (SP-4-2)- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN

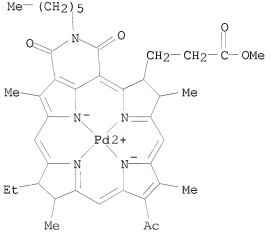
ACCESSION NUMBER:	2008:153213 CAPLUS <<LOGINID::20081001>>
DOCUMENT NUMBER:	148:390704
TITLE:	Metal Bacteriochlorins Which Act as Dual Singlet Oxygen and Superoxide Generators
AUTHOR(S):	Fukuzumi, Shunichi; Ohkubo, Kei; Zheng, Xiang; Chen, Yihui; Pandey, Ravindra K.; Zhan, Riqiang; Kadish, Karl M.
CORPORATE SOURCE:	Department of Material and Life Science, Graduate School of Engineering, Osaka University, Suita, Osaka, 565-0871, Japan
SOURCE:	Journal of Physical Chemistry B (2008), 112(9), 2738-2746 CODEN: JPCBFK; ISSN: 1520-6106
PUBLISHER:	American Chemical Society
DOCUMENT TYPE:	Journal
LANGUAGE:	English

AB A series of stable free-base, ZnII and PdII bacteriochlorins containing a

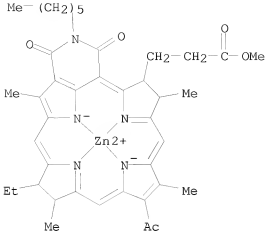
fused six- or five-member diketo- or imide ring have been synthesized as good candidates for photodynamic therapy sensitizers, and their electrochem., photophys., and photochem. properties were examined Photoexcitation of the palladium bacteriochlorin affords the triplet excited state without fluorescence emission, resulting in formation of singlet oxygen with a high quantum yield due to the heavy atom effect of palladium. Electrochem. studies revealed that the zinc bacteriochlorin has the smallest HOMO-LUMO gap of the investigated compds., and this value is significantly lower than the triplet excited-state energy of the compound in benzonitrile. Such a small HOMO-LUMO gap of the zinc bacteriochlorin enables intermol. photoinduced electron transfer from the triplet excited state to the ground state to produce both the radical cation and the radical anion. The radical anion thus produced can transfer an electron to mol. oxygen to produce superoxide anion which was detected by ESR. The same photosensitizer can also act as an efficient singlet oxygen generator. Thus, the same zinc bacteriochlorin can function as a sensitizer with a dual role in that it produces both singlet oxygen and superoxide anion in an aprotic solvent (benzonitrile).

IT 1014695-22-7P 1014695-23-8P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(photochem./photophys. and electrochem. properties of free-base and metal bacteriochlorins as dual superoxide and singlet oxygen generators)

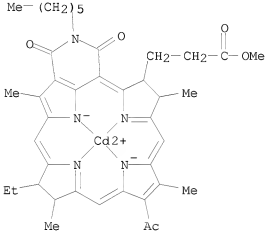
RN 1014695-22-7 CAPLUS
CN Palladium, [methyl (5R,6R,15S,16S)-10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-9,12-imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoato(2-)-κN1,κN23,κN24,κN25]-, (SP-4-2)-
(CA INDEX NAME)



RN 1014695-23-8 CAPLUS
CN Zinc, [methyl (5R,6R,15S,16S)-10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-9,12-imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoato(2-)-κN1,κN23,κN24,κN25]-, (SP-4-2)-
(CA INDEX NAME)

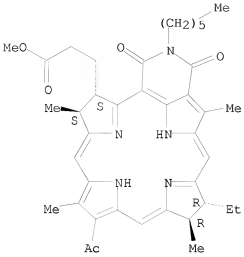


IT 1014695-27-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(photochem./photophys. and electrochem. properties of free-base and metal bacteriochlorins as dual superoxide and singlet oxygen generators)
RN 1014695-27-2 CAPLUS
CN Cadmium, [methyl (5R,6R,15S,16S)-10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-9,12-imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoato(2-)-κN1,κN23,κN24,κN25]-, (SP-4-2)-
(CA INDEX NAME)



IT 952186-20-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of metal bacteriochlorins as dual superoxide and singlet oxygen generators)
RN 952186-20-8 CAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:1004165 CAPLUS <<LOGINID::20081001>>

DOCUMENT NUMBER: 147:486250

TITLE: Conversion of bacteriochlorophyll-a to bacteriopurpurin-18: A useful synthon for the construction of bioactive agents for photodynamic therapy (PDT)

AUTHOR(S): Goswami, Lalit N.; Chen, Yihui; Missert, Joseph; Li, Guolin; Pallenberg, Alex; Pandey, Ravindra K.

CORPORATE SOURCE: Medicinal Chemistry Division, Photodynamic Therapy Center, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA

SOURCE: Heterocycles (2007), 71(9), 1929-1949
CODEN: HTCYAM; ISSN: 0385-5414

PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:486250

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Bacteriochlorophyll-a I (R = Q) present in Rb. sphaeroides was converted into bacteriopurpurin-18 Me ester II (X = O) (III) by following three different approaches and was used as a substrate for the preparation of a series of stable bacteriochlorins with long wavelength absorptions ranging from 760 to 824 nm. Bacteriopurpurin p6 IV (R1 = R2 = CO2H), obtained by the base hydrolysis of III, on reacting with L-aspartyl-di-tert-Bu ester in presence of EDCI and DMAP afforded the corresponding N-aspartyl-bacteriopurpurinimide II [X = NCH(CO2CMe3)CH2CO2CMe3] (V) in high yield, possibly by the base-catalyzed intramol. cyclization via imide

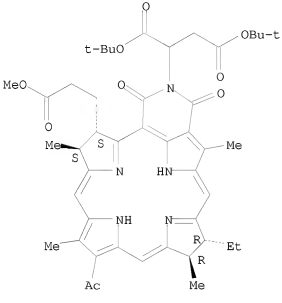
intermediate(s). A possible mechanism for the formation of III and bacteriochlorin 15-glyoxylic acid tri-Me ester IV (R1 = CO2Me, R2 = COCO2Me) from I via a hydroxylactone is also discussed. Among the compds. synthesized, the bacteriochlorin V containing a fused cyclic imide ring system was found to be the most stable in various solvents at room temperature and exhibited the longest wavelength absorption at 824 nm in dichloromethane.

IT 953795-68-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and absorption spectra of bacteriopurpurin-18 Me ester and derivs. for potential use in photodynamic therapy)

RN 953795-68-1 CAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16,19(20H)-dipropanoic acid, 10-acetyl-β19-[(1,1-dimethylethoxy)carbonyl]-5-ethyl-1,5,6,15,16,18-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, 19-(1,1-dimethylethyl) 16-methyl ester, (5R,6R,15S,16S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:914597 CAPLUS <<LOGINID::20081001>>

DOCUMENT NUMBER: 147:442644

TITLE: Comparative in Vitro and in Vivo Studies on Long-Wavelength Photosensitizers Derived from Bacteriopurpurinimide and Bacteriochlorin p6: Fused Imide Ring Enhances the in Vivo PDT Efficacy

AUTHOR(S): Chen, Yihui; Potter, William R.; Missert, Joseph R.; Morgan, Janet; Pandey, Ravindra K.

CORPORATE SOURCE: Medicinal Chemistry Division, PDT Center and Department of Dermatology, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA

SOURCE: Bioconjugate Chemistry (2007), 18(5), 1460-1473
CODEN: BCCHES; ISSN: 1043-1802

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:442644

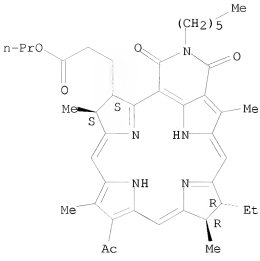
AB In situ conversion of bacteriochlorophyll-a, present in Rhodobacter sphaeroides (Rb. sphaeroides) gave bacteriopurpurin-18 in modest yield, which in a sequence of reactions was converted into two series of bacteriochlorins: bacteriopurpurinimide and bacteriopurpurin p6 with and without a fused imide ring system, resp. To determine the effect of overall lipophilicity in photosensitizing efficacy, these bacteriochlorins were independently reacted with HBr gas and subsequently treated with various alkyl alcs. to afford the corresponding alkyl ether derivs. as diastereomeric mixts. (the R- and S-isomers were obtained in almost equal ratios). Between the two series of bacteriochlorins, the bacteriopurpurinimides containing a fused imide ring system were found to be more effective in vivo (C3H mice bearing RIF tumors). To investigate the effect of the presence of the chiral center at position 3 of the most effective purpurinimide 9 [3(1'-heptyloxy)ethyl-3-deacetyl-bacteriopurpurin-18-N-hexylimide Pr ester], the acetyl group was replaced with a hydroxymethyl substituent and converted into 3(1'-decyloxy)methyl-3-deacetyl-purpurin-18-N-hexylimide Me ester 26 with a similar lipophilicity. Interestingly, compared to 26, the bacteriopurpurinimide 9 was found to be more effective, suggesting that the chiral center at position 3 certainly plays an important role in photosensitizing activity. Among a series of alkyl ether analogs, between the PDT efficacy and the lipophilicity (log P and log D) calculated by computational methods (PALLAS program), a parabolic relationship was observed to some extent. However, it was limited to a particular series, e.g., compds. with similar log P values between bacteriopurpurinimides and bacteriochlorin e6 did not produce similar in vivo efficacy. As expected, within a series, a linear relationship was observed between the log P values and the HPLC retention times of the photosensitizers. Some of the mitochondrial localized photosensitizers showed a significant peripheral benzodiazepine binding (PBR) affinity. However, limited correlation between PBR binding affinity and in vivo PDT efficacy was observed Compared to the naturally occurring bacteriochlorophyll-a, the bacteriopurpurinimides with fused imide ring system showed higher in vitro/in vivo stability. In contrast to Me pyropheophorbide-a, the ester functionalities in bacteriopurpurinimide did not convert into the corresponding carboxylic acid by the enzyme esterases.

IT 182253-28-7P 952186-20-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(fused imide ring enhances the in vivo PDT efficacy of long-wavelength photosensitizers derived from bacteriopurpurinimide and bacteriochlorin p6)

RN 182253-28-7 CAPLUS

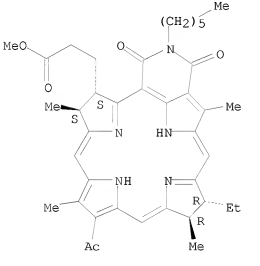
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 952186-20-8 CAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (CA INDEX NAME)

Absolute stereochemistry.

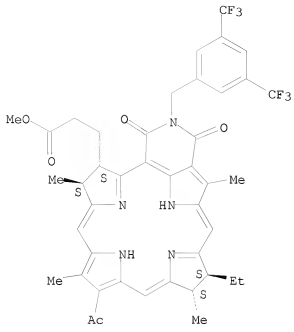


REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:316707 CAPLUS <<LOGINID::20081001>>
DOCUMENT NUMBER: 146:517111
TITLE: Structure-Activity Relationship Among Purpurinimides and Bacteriopurpurinimides: Trifluoromethyl Substituent Enhanced the Photosensitizing Efficacy
AUTHOR(S): Gryshuk, Amy; Chen, Yihui; Goswami, Lalit N.; Pandey, Suresh; Missert, Joseph R.; Ohulchanskyy, Tymish;

Potter, William; Prasad, Paras N.; Oseroff, Allan; Pandey, Ravindra K.
CORPORATE SOURCE: Chemistry Division, PDT Center and Department of Dermatology, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA
SOURCE: Journal of Medicinal Chemistry (2007), 50(8), 1754-1767
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:517111
AB At similar lipophilicity, compared to the nonfluorinated purpurinimide 11, the corresponding fluorinated analog 8 with a trifluoromethyl substituent at the lower half (position-132) of the mol. showed enhanced photosensitizing efficacy. The structural parameters established in purpurinimides (λmax: 700 nm) were successfully translated to the bacteriopurpurin imide system 19 (λmax: 792 nm) and within both series, a monotonic relationship between the lipophilicity and the in vivo PDT activity was observed For preparing water-soluble compds., the photosensitizers 8 and 19 were converted into the corresponding aminobenzyl-diethylenetriamine pentaacetate conjugates 23 and 26. Acid treatment of purpurinimide 23 produced the corresponding water-soluble analog 24. Bacteriochlorin 26 under acidic or basic conditions mainly gave the decomposition products. At similar in vivo treatment conditions (C3H mice with RIF tumors and BALB-C mice with colon-26 tumors) the water-soluble purpurinimide 24 was found to be more effective than the Me ester analog 8. These results suggest that besides overall lipophilicity the inherent charge of the photosensitizer also influences the PDT efficacy.
IT 936639-75-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(SAR among purpurinimides and bacteriopurpurinimides: trifluoromethyl substituent enhanced photosensitizing efficacy)
RN 936639-75-7 CAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5S,6S,15S,16S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:199779 CAPLUS <<LOGINID::20081001>>
DOCUMENT NUMBER: 148:195138
TITLE: Preparation and application of long-life charge separation system
AUTHOR(S): Fukuzumi, Shunichi
CORPORATE SOURCE: Grad. Sch. of Engineering, OORST, Osaka Univ., Osaka, Japan
SOURCE: TCIMeru (2007), 133, 2-13
CODEN: TCIMCV; ISSN: 1349-4856
PUBLISHER: Tokyo Kasei Kogyo
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

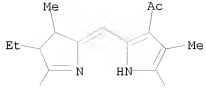
AB This paper introduces application development of a photocatalyst reaction system using a connecting mol. as a photocatalyst which generates a high-energy and long-life charge separation state, and summarizes recent results on preparation and application of a long-life charge separation system in an artificial photosynthesis study.

IT 478978-75-5
RL: TEM (Technical or engineered material use); USES (Uses)
(preparation and application of long-life charge separation systems)

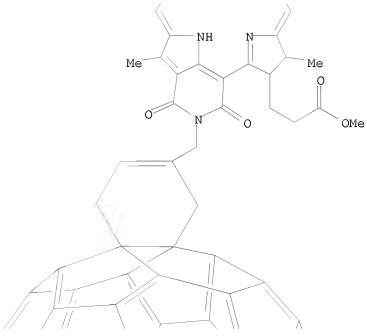
RN 478978-75-5 CAPLUS

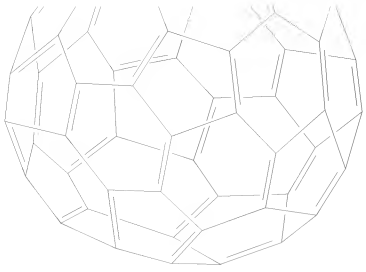
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-19-[(3',6'-dihydrobenzo[1,9][5,6]fulleren-C60-Ih-4'-yl)methyl]-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15-trimethyl-18,20-dioxo-, methyl ester, (5S,6S,15S,16S)- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A





L4 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:153085 CAPLUS <<LOGINID::20081001>>
DOCUMENT NUMBER: 144:365450
TITLE: In Vivo Stability and Photodynamic Efficacy of Fluorinated Bacteriopurpurinimides Derived from Bacteriochlorophyll-a
AUTHOR(S): Gryshuk, Amy L.; Chen, Yihui; Potter, William; Ohulchansky, Tymish; Oseroff, Allan; Pandey, Ravindra K.
CORPORATE SOURCE: Photodynamic Therapy Center, Department of Dermatology and Department of Nuclear Medicine/Radiology, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA
SOURCE: Journal of Medicinal Chemistry (2006), 49(6), 1874-1881
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:365450

AB The stable bacteriopurpurinimide (788 nm, ε: 38 600 in CH2Cl2), obtained by reducing the corresponding unstable Schiff base (803 nm, ε: 50 900 in CH2Cl2) that was isolated by reacting bacteriopurpurin Me ester with 3,5-bis-(trifluoromethyl)benzylamine, produced promising photosensitizing efficacy. 1H NMR, mass spectrometry, and HPLC analyses confirmed the structures of new bacteriopurpurinimides and the metabolic product. The preliminary in vivo photosensitizing efficacy of this stable bacteriopurpurinimide was determined in C3H mice bearing radiation induced fibrosarcoma tumors as a function of variable drug doses. A drug dose of 1.0 μmol/kg and light exposure of 135 J/cm2 (75 mW/cm2; 24 h postinjection) at 796 nm for 30 min produced a 60% long-term tumor cure (3/5 mice were tumor-free on day 90). Colocalization study of the stable bacteriopurpurinimide with MitoTracker Green confirmed some mitochondrial localization. The fluorescein-exclusion assay and histol. staining of CD31 confirmed vascular stasis at various time points post-PDT (post photodynamic therapy). The treatment parameters (time for maximum drug uptake and wavelength for light irradiation) were determined by in vivo

reflectance spectroscopy.

IT 639857-54-8P

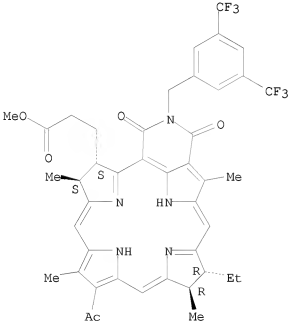
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(in vivo stability and photodynamic efficacy of fluorinated bacteriopurpurinimides derived from bacteriochlorophyll-a)

RN 639857-54-8 CAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:122072 CAPLUS <<LOGINID::20081001>>

DOCUMENT NUMBER: 144:369794

TITLE: Characterization of porphyrins, chlorins, and bacteriochlorins formed via allomerization ofbBacteriochlorophyll a. synthesis of highly stable bacteriopurpurinimides and their metal complexes

AUTHOR(S): Kozyrev, Andrei N.; Chen, Yihui; Goswami, Lalit N.; Tabaczynski, Walter A.; Pandey, Ravindra K.

CORPORATE SOURCE: Chemistry Division, PDT Center, Cell Stress Biology, NMR Facility, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA

SOURCE: Journal of Organic Chemistry (2006), 71(5), 1949-1960 CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:369794

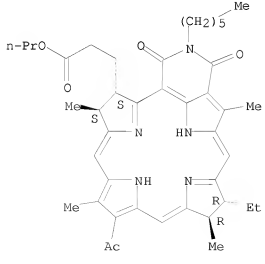
AB Allomerization of bacteriochlorophyll a (Bchl a) was studied under various reaction conditions. Bchl a on stirring with KOH/propanol produced an "unstable bacteriochlorin", which decomposed in acidic conditions to give a complex mixture containing bacteriopurpurin a as a principal component. The yields of other compds. varied and were found to be dependent on reaction condition. The structures of the isolated porphyrins, chlorins, and bacteriochlorins, related to Bchl a, were assigned on the basis of 1D, 2D NMR (ROESY), and mass spectroscopy analyses. The presence of fused anhydride rings in porphyrin, chlorin, and bacteriochlorin systems showed a significant influence on their optical properties. Compared to bacteriochlorophyll a and bacteriopheophytin, the related structurally modified analogs, e.g., the bacteriopurpurin a, 131/151-N-alkyl isoimide, and the imide analogs were found to be more stable with a significant difference in spectroscopic properties. Bacteriochlorins containing anhydride, imide, or isoimide cyclic rings demonstrated a significant bathochromic shift of their Q bands in their electronic absorption spectra. Under basic conditions the formation of the 12-hydroxymethyl, 12-formyl, and 12-methylene analogs as byproducts from the 12-methyl-bacteriopurpurin-N-hexylimide could be due to subsequent oxidation of the vinylogous enolate intermediates. To investigate the effect of the central metal in the electronic spectra, the stable bacteriopurpurin-18-N-hexylimide was converted to a series of metal complexes [Zn(II), Cd(II), and Pd(II)] by following the direct or transmetalation approaches. Compared to the free-base analog, these complexes showed a remarkable shift in their electronic absorption spectra.

IT 182253-28-7P 881683-27-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(characterization of porphyrins, chlorins, and bacteriochlorins formed via allomerization of bacteriochlorophyll a)

RN 182253-28-7 CAPLUS

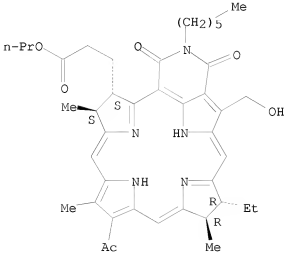
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (CA INDEX NAME)

Absolute stereochemistry.



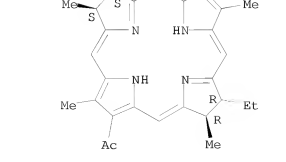
RN 881683-27-8 CAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-22-(hydroxymethyl)-6,11,15-trimethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



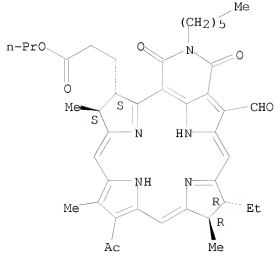
IT 881683-26-7P 881683-29-0P 881683-45-0P
882006-45-3P 882006-46-4P 882006-47-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(characterization of porphyrins, chlorins, and bacteriochlorins formed via allomerization of bacteriochlorophyll a)
RN 881683-26-7 CAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,19,22-pentamethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



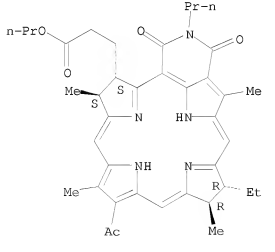
RN 881683-29-0 CAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-22-formyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15-trimethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



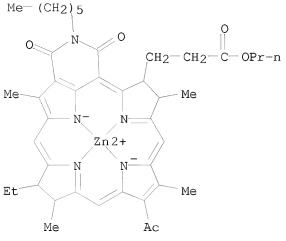
RN 881683-45-0 CAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-19-propyl-, propyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

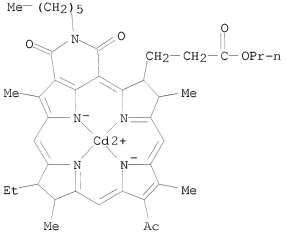


RN 882006-45-3 CAPLUS
CN Zinc, [propyl (5R,6R,15S,16S)-10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-9,12-

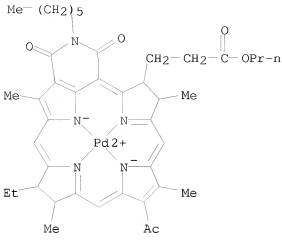
imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoato(2-)-κN1,κN23,κN24,κN25]-, (SP-4-2)-
(9CI) (CA INDEX NAME)



RN 882006-46-4 CAPLUS
CN Cadmium, [propyl (5R,6R,15S,16S)-10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-9,12-imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoato(2-)-κN1,κN23,κN24,κN25]-, (SP-4-2)-
(9CI) (CA INDEX NAME)



RN 882006-47-5 CAPLUS
CN Palladium, [propyl (5R,6R,15S,16S)-10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-9,12-imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoato(2-)-κN1,κN23,κN24,κN25]-, (SP-4-2)-
(9CI) (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:510479 CAPLUS <<LOGINID::20081001>>
DOCUMENT NUMBER: 143:168789
TITLE: Investigation of human serum albumin (HSA) binding specificity of certain photosensitizers related to pyropheophorbide-a and bacteriopurpurinimide by circular dichroism spectroscopy and its correlation with in vivo photosensitizing efficacy
AUTHOR(S): Chen, Yihui; Miclea, Razvan; Srikrishnan, Thamarapu; Balasubramanian, Sathyamangalam; Dougherty, Thomas J.; Pandey, Ravindra K.
CORPORATE SOURCE: Chemistry Division, Photodynamic Therapy Center, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(13), 3189-3192
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

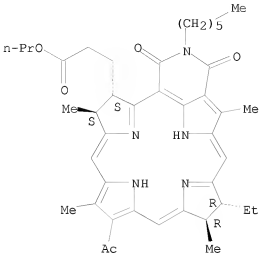
AB A series of pyropheophorbide-a and bacteriopurpurinimides were investigated to understand the correlation between HSA (site II) binding affinity and in vivo photosensitizing activity. In our study, photosensitizers that bound to site II of HSA produced a significant difference in the CD spectra of the corresponding complexes, especially at Soret band region of the photosensitizers. Our results suggest that CD spectroscopy of the photosensitizer-HSA complexes could be a valuable tool in screening new photosensitizers before evaluating them for in vivo efficacy.

IT 182253-28-7
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(HSA-binding specificity of photosensitizers, its correlation with photosensitizing efficacy, and CD spectroscopy use for screening)

RN 182253-28-7 CAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, propyl

ester, (5R,6R,15S,16S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:470253 CAPLUS <<LOGINID::20081001>>
DOCUMENT NUMBER: 143:32213
TITLE: Activatable photodynamic therapy agents
INVENTOR(S): Zheng, Gang; Glickson, Jerry D.; Chance, Britton; Delikatny, Edward James
PATENT ASSIGNEE(S): University of Pennsylvania, USA
SOURCE: PCT Int. Appl., 92 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005048944	A2	20050602	WO 2004-US38024	20041115
WO 2005048944	A3	20060504		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20080193431	A1	20080814	US 2006-383487	20060515
PRIORITY APPLN. INFO.:			US 2003-519794P P	20031114
			US 2004-558501P P	20040401

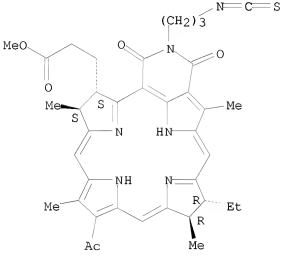
AB The present invention relates to the field of conjugates comprising a first substrate which is attached to a least one photosensitizer and at least one first quencher, and methods for their use. More particularly, the present invention relates to photodynamic therapy agents. The substrate is cleavable by enzymes associated with diseases or infective/contaminating agents such as retroviral proteases. The invention further relates to methods for decontaminating blood and methods for treating cancer or viral infection in a subject using the conjugates of the present invention.

IT 810676-12-1P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(enzyme-cleavable photosensitizer quencher peptide conjugates for photodynamic blood decontamination and therapy)

RN 810676-12-1 CAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-1,5,6,15,16,18,19,20-octahydro-19-(3-isothiocyanatopropyl)-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:1124548 CAPLUS <<LOGINID::20081001>>
DOCUMENT NUMBER: 142:56618
TITLE: Preparation of 2-aminodeoxy-glucose derivatives as antineoplastic agents targeted via GLUT transporters
INVENTOR(S): Zheng, Gang; Glickson, Jerry D.; Chance, Britton
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 71 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004110255	A2	20041223	WO 2004-US18143	20040609
WO 2004110255	A3	20051027		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 20060171893	A1	20060803	US 2005-560075		20051209
PRIORITY APPLN. INFO.:			US 2003-476648P	P	20030609
			US 2004-537282P	P	20040116
			US 2004-540700P	P	20040130
			US 2004-548240P	P	20040227
			WO 2004-US18143	W	20040609

OTHER SOURCE(S): MARPAT 142:56618
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention relates to novel antineoplastic agents and cancer diagnostic agents that specifically target neoplastic cells via the GLUT transportation system. More specifically, the invention relates to conjugates of 2-deoxyglucose I, wherein L is a linker, which includes a covalent bond, is attached to 2-deoxyglucose at the 2 position, and the linker is attached to a therapeutic or diagnostic agent D, provided that D is not (18F)deoxyglucose or 2-[N-(7-nitrobenz-2-oxa-1,3-diazol-4-yl)amino]-2-deoxy-D-glucose. The invention also relates to methods of treating tumor disease and methods of making the novel compds. of the present invention. The agents of the present invention are superior to previous agents as they are targeted via GLUT transporters. In vivo tumor detection was realized by optical imaging. One of the 2-deoxyglucose conjugates of [bacteriochlorophyl](BChlPP-2DG) was imaged in vivo on an animal model of human cancer. The synthesis of two novel functionalized bacteriochlorophylls dyes is described. These functionalized bacteriochlorophylls showed successful conjugation to the glucose transporter-homing 2-deoxyglucose moiety. Thus, 2-aminodeoxy-glucose derivative II was prepared and tested in mice as antineoplastic agent targeted via GLUT transporter.

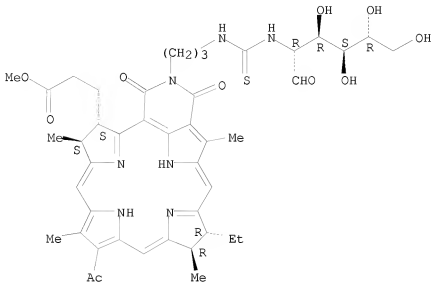
IT 810676-14-3P
RL: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-aminodeoxy-glucose derivs. as antineoplastic agents targeted via GLUT transporters)

RN 810676-14-3 CAPLUS

CN D-Glucose, 2-[[[[3-[(5R,6R,15S,16S)-10-acetyl-5-ethyl-1,5,6,15,16,18-hexahydro-16-(3-methoxy-3-oxopropyl)-6,11,15,22-tetramethyl-18,20-dioxo-9,12-imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-

b]azacyclononadecin-19(20H)-yl]propyl]amino]thioxo]amino]-2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

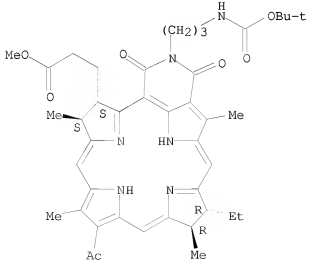


IT 810676-08-5P 810676-10-9P 810676-12-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-aminodeoxy-glucose derivs. as antineoplastic agents targeted via GLUT transporters)

RN 810676-08-5 CAPLUS

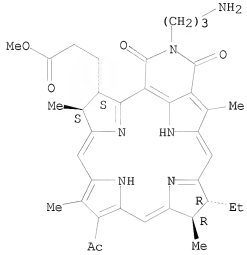
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-19-[3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



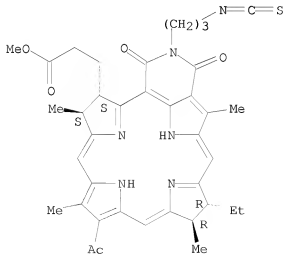
RN 810676-10-9 CAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-19-(3-aminopropyl)-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

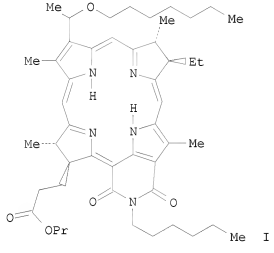


RN 810676-12-1 CAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-1,5,6,15,16,18,19,20-octahydro-19-(3-isothiocyanatopropyl)-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:704822 CAPLUS <<LOGINID::20081001>>
DOCUMENT NUMBER: 141:366057
TITLE: Synthesis and photosensitizing efficacy of isomerically pure bacteriopurpurinimides
AUTHOR(S): Chen, Yihui; Sumlin, Adam; Morgan, Janet; Gryshuk, Amy; Oseroff, Allan; Henderson, Barbara W.; Dougherty, Thomas J.; Pandey, Ravindra K.
CORPORATE SOURCE: PDT Center, Department of Dermatology and Department of Nuclear Medicine/Radiology, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA
SOURCE: Journal of Medicinal Chemistry (2004), 47(20), 4814-4817
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:366057
GI



I

AB The isometrically pure 3-deacetyl-3-(1-heptyloxy)ethylbacteriopurpurin-N-hexylimides I exhibiting long-wavelength absorption near 800 nm were obtained from 3-acetylbacteriopurpurin-N-hexylimide in high stereospecificity by following Corey's synthetic approach. Both heptyl ether derivs. (R- and S-isomers) showed similar in vitro photosensitizing efficacy and limited skin phototoxicity and were found to localize in mitochondria. However, in preliminary in vivo screening, compared to the S-isomer, the corresponding R-isomer produced enhanced in vivo photodynamic therapy efficacy.

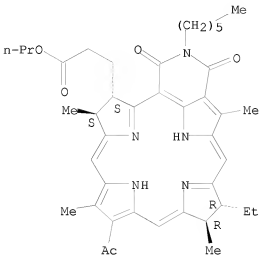
IT 182253-28-7P
RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and photosensitizing efficacy of isomerically pure bacteriopurpurinimides)

RN 182253-28-7 CAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-

b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:20489 CAPLUS <<LOGINID::20081001>>
DOCUMENT NUMBER: 140:73251
TITLE: Fluorinated photosensitizers related to chlorins and bacteriochlorins for photodynamic therapy
INVENTOR(S): Pandey, Ravindra K.; Potter, William R.; Dougherty, Thomas J.
PATENT ASSIGNEE(S): Health Research, Inc., USA
SOURCE: PCT Int. Appl., 120 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004002476	A2	20040108	WO 2003-US20427	20030627
WO 2004002476	A9	20040401		
WO 2004002476	A3	20040513		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2490692	A1	20040108	CA 2003-2490692		20030627
AU 2003248747	A1	20040119	AU 2003-248747		20030627
EP 1517684	A2	20050330	EP 2003-762180		20030627

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

PRIORITY APPLN. INFO.: US 2002-392473P P 20020627
WO 2003-US20427 W 20030627

OTHER SOURCE(S): MARPAT 140:73251

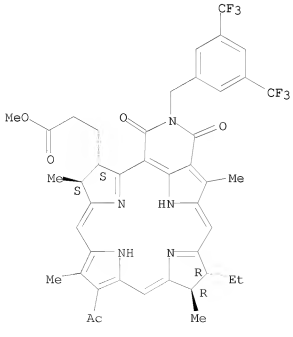
AB Provided herein are compds. for detection, diagnosis and treatment of target tissues or target compns., including hyperproliferative tissues such as tumors, using photodynamic methods. In particular, photosensitizer compds. that collect in hyperproliferative tissue are provided. In another embodiment, compds. that absorb light at a wavelength of from about 700 to about 850 nm are provided. In a further embodiment, compds. that are detectable by magnetic resonance imaging are provided. Among examples provided are preparation of purpurinimides and their potential photodynamic efficacy against tumor cells, against Helicobacter pylori, against pulmonary tuberculosis, and against otitis media.

IT 639857-54-8P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(fluorinated photosensitizers related to chlorins and bacteriochlorins for photodynamic therapy)

RN 639857-54-8 CAPLUS

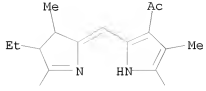
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

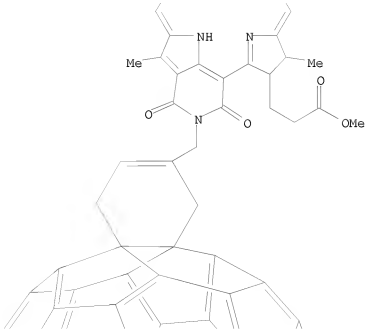


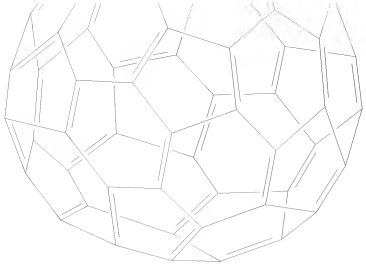
L4 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:683489 CAPLUS <<LOGINID::20081001>>
DOCUMENT NUMBER: 140:50149
TITLE: Intramolecular electron transfer in bacteriochlorin-C60 and zinc chlorin-C60 dyads
AUTHOR(S): Ohkubo, Kei; Imahori, Hiroshi; Shao, Jianguo; Ou, Zhongping; Kadish, Karl M.; Chen, Yihui; Zheng, Gang; Pandey, Ravindra K.; Fujitsuka, Mamoru; Ito, Osamu; Fukuzumi, Shunichi
CORPORATE SOURCE: Department of Material and Life Science, Graduate School of Engineering, CREST, Japan Science and Technology Corporation, Osaka University, Osaka, 565-0871, Japan
SOURCE: Proceedings - Electrochemical Society (2002), 2002-12(Fullerenes--Volume 12: The Exciting World of Nanocages and Nanotubes), 70-81
CODEN: PESODO; ISSN: 0161-6374
PUBLISHER: Electrochemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Rate consts. for charge separation (CS) processes in free base bacteriochlorin- and zinc chlorin-C60 dyads were determined by fluorescence lifetime measurements of the dyads. The charge recombination (CR) rate consts. of the dyads were determined using laser flash photolysis. Photoexcitation of the zinc chlorin-C60 dyad results in formation of long-lived radical ion pair which has absorption maxima at 790 and 1000 nm due to the zinc chlorin radical cation and the C60 radical anion, resp. Photoexcitation of the free-base bacteriochlorin-C60 dyad with the same short linkage leads to formation of the radical ion pair which decays quickly to the triplet excited state of the bacteriochlorin moiety. The driving force dependence of the electron transfer rate consts. of the dyads with a short spacer affords a small reorganization energy (λ) compared with the λ value of zinc porphyrin-C60 dyads with longer spacers.
IT 478978-75-5
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(dyad; photochem. and electrochem. study of free base bacteriochlorin-C60 and zinc chlorin-C60 dyads)
RN 478978-75-5 CAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-19-[(3',6'-dihydrobenzo[1,9][5,6]fulleren-C60-Ih-4'-yl)methyl]-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15-trimethyl-18,20-dioxo-, methyl ester, (5S,6S,15S,16S)- (CA INDEX NAME)

PAGE 1-A



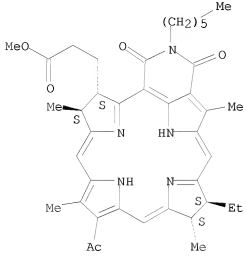
PAGE 2-A





IT 438627-03-3
RL: PRP (Properties)
(reference compound; photochem. and electrochem. study of free base bacteriochlorin-C60 and zinc chlorin-C60 dyads)
RN 438627-03-3 CAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-1,5,6,15,16,18,19,20-octahydro-5-ethyl-19-hexyl-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5S,6S,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:801953 CAPLUS <<LOGINID::20081001>>
DOCUMENT NUMBER: 138:47144

TITLE: Small Reorganization Energy of Intramolecular Electron Transfer in Fullerene-Based Dyads with Short Linkage

AUTHOR(S): Ohkubo, Kei; Imahori, Hiroshi; Shao, Jianguo; Ou, Zhongping; Kadish, Karl M.; Chen, Yihui; Zheng, Gang; Pandey, Ravindra K.; Fujitsuka, Mamoru; Ito, Osamu; Fukuzumi, Shunichi

CORPORATE SOURCE: Department of Material and Life Science Graduate School of Engineering, Osaka University, Osaka, 565-0871, Japan

SOURCE: Journal of Physical Chemistry A (2002), 106(46), 10991-10998
CODEN: JPCAFH; ISSN: 1089-5639

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

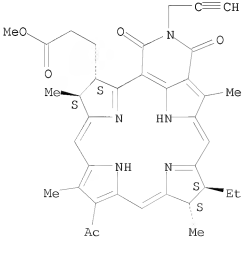
AB A bacteriochlorin-C60 dyad (H2BCh-C60) and a zinc chlorin dyad (ZnCh-C60) with the same short spacer have been synthesized. The rate consts. for the charge-separation (CS) processes in these dyads were determined by fluorescence lifetime measurements of the dyads. The charge-recombination (CR) rate consts. of the dyads were determined using laser flash photolysis. The photoexcitation of the zinc chlorin-C60 dyad results in formation of the long-lived radical ion pair, which has absorption maxima at 790 and 1000 nm due to the zinc chlorin radical cation and the C60 radical anion, resp. Photoexcitation of the free-base bacteriochlorin-C60 dyad with the same short linkage leads to formation of the radical ion pair, which decays quickly to the triplet excited state of the bacteriochlorin moiety. The driving force dependence of the electron-transfer rate consts. of these dyads with a short spacer affords a small reorganization energy (λ = 0.51 eV) as compared with the λ value (0.66 eV) of zinc porphyrin-C60 dyads with a longer spacer.

IT 478945-66-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in synthesis of bacteriochlorin fullerene dyad)

RN 478945-66-3 CAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-19-(2-propynyl)-, methyl ester, (5S,6S,15S,16S)- (9CI) (CA INDEX NAME)

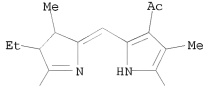
Absolute stereochemistry.



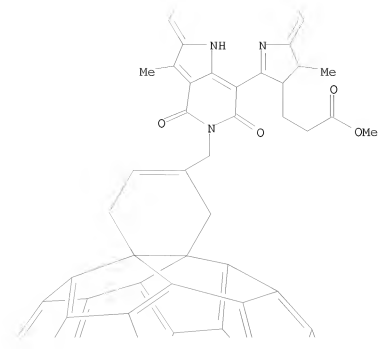
IT 478978-75-5P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(photochem. and electrochem. properties of free base bacteriochlorin- and zinc chlorin-fullerene dyads)

RN 478978-75-5 CAPLUS

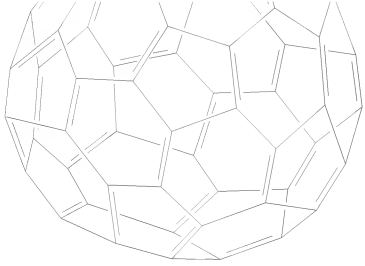
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-19-[(3',6'-dihydrobenzo[1,9][5,6]fulleren-C60-Ih-4'-yl)methyl]-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15-trimethyl-18,20-dioxo-, methyl ester, (5S,6S,15S,16S)- (CA INDEX NAME)



PAGE 2-A



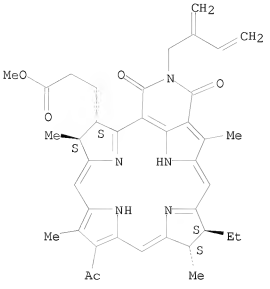
PAGE 3-A



IT 478945-67-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction with C60 in synthesis of bacteriochlorin fullerene dyad)
RN 478945-67-4 CAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-19-(2-methylene-3-butenyl)-18,20-dioxo-, methyl ester, (5S,6S,15S,16S)- (9CI) (CA INDEX

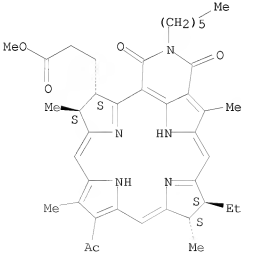
NAME)

Absolute stereochemistry.



IT 438627-03-3
RL: PRP (Properties)
(reference compound; photochem. and electrochem. properties of free base bacteriochlorin- and zinc chlorin-fullerene dyads)
RN 438627-03-3 CAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-1,5,6,15,16,18,19,20-octahydro-5-ethyl-19-hexyl-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5S,6S,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS

L4 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:287224 CAPLUS <<LOGINID::20081001>>
DOCUMENT NUMBER: 137:63096
TITLE: Photophysical and Electrochemical Properties of New Bacteriochlorins and Characterization of Radical Cation and Radical Anion Species
AUTHOR(S): Fukuzumi, Shunichi; Ohkubo, Kei; Chen, Yihui; Pandey, Ravindra K.; Zhan, Riqiang; Shao, Jianguo; Kadish, Karl M.
CORPORATE SOURCE: Department of Material and Life Science, Graduate School of Engineering, Osaka University, Suita, Osaka, 565-0871, Japan
SOURCE: Journal of Physical Chemistry A (2002), 106(20), 5105-5113
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:63096

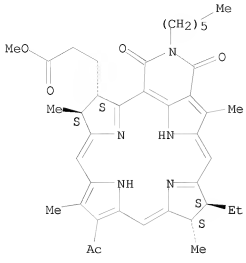
AB The synthesis, photophys., and photochem. properties of a series of stable bacteriochlorins containing a fused six-member anhydride or an imide ring are discussed. The Qy band (alu → egx transition) in the near-IR region (NIR) lies between 788 and 831 nm depending upon the macrocycle substituents. Compds. with such a long-wavelength absorption are highly promising for their potential use in photodynamic therapy. Fluorescence maxima are also observed in the long-wavelength region of the spectrum, between 804 and 842 nm, and have lifetimes between 1.1 and 1.4 ns. The phosphorescence maxima are red-shifted to 840-870 nm. The triplet-triplet transient absorption spectra are observed to have maxima between 570 and 640 nm with lifetimes between 72 and 150 μs. The triplet excited states are efficiently quenched by oxygen to produce singlet oxygen. The quantum yields of the generated singlet oxygen were determined to be in the range of 0.33-0.55. The bacteriochlorin derivs. are easy to oxidize by one electron, and reversible half-wave potentials range between 0.65 and 0.82 V vs. SCE in benzonitrile containing 0.1 M tetra-n-butylammonium perchlorate (TBAP). The second oxidation is irreversible and occurs at a rather constant potential of 1.17-1.22 V independent of the macrocycle substituents. The bacteriochlorin derivs. are also easy to reduce, and the reversible first and second one-electron reduction potentials range between -0.53 and -0.80 V and between -0.95 and -1.28 V vs. SCE, resp. Spectroelectrochem. measurements reveal the expected π radical cation and π radical anion marker bands of the bacteriochlorin derivs. The ESR spectra of the radical cations and radical anions produced by the chemical oxidation and reduction are reported, and the exptl. and calculated spin densities are compared to each other.

IT 438627-03-3P
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(intermediate/product/bacteriochlorin analog; preparation and photophys. and electrochem. properties of bacteriochlorin analogs containing fused 6-membered anhydride or imide ring in relation to photosensitizer use)

RN 438627-03-3 CAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-1,5,6,15,16,18,19,20-

octahydro-5-ethyl-19-hexyl-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5S,6S,15S,16S)- (9CI) (CA INDEX NAME)

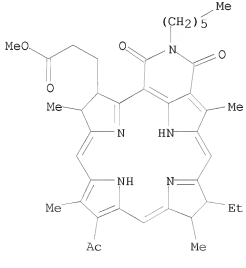
Absolute stereochemistry.



IT 439090-20-7 439097-71-9
RL: PRP (Properties)
(photophys. properties of radical anions and cations of bacteriochlorin analogs containing fused 6-membered anhydride or imide ring)

RN 439090-20-7 CAPLUS

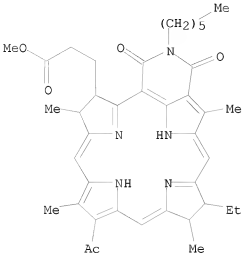
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, radical ion(1-), (5S,6S,15S,16S)- (9CI) (CA INDEX NAME)



RN 439097-71-9 CAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-19-hexyl-

1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, radical ion(1+), (5S,6S,15S,16S)- (9CI) (CA INDEX NAME)

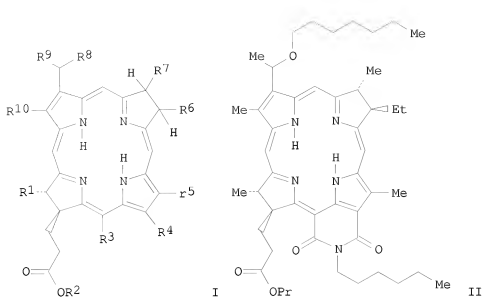


REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:918882 CAPLUS <<LOGINID::20081001>>
DOCUMENT NUMBER: 136:37447
TITLE: Long wavelength absorbing bacteriochlorin alkyl ether analogs for the treatment and detection of hyperproliferative tissues such as tumors using photodynamic methods.
INVENTOR(S): Pandey, Ravindra K.; Dougherty, Thomas J.; Potter, William R.
PATENT ASSIGNEE(S): Health Research, Inc., USA
SOURCE: Eur. Pat. Appl., 18 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1164136	A1	20011219	EP 2001-108984	20010411
EP 1164136	B1	20040609		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 6624187	B1	20030923	US 2000-592150	20000612
CA 2342064	A1	20011212	CA 2001-2342064	20010321
AT 268777	T	20040615	AT 2001-108984	20010411
JP 2002020389	A	20020123	JP 2001-116889	20010416

PRIORITY APPLN. INFO.: US 2000-592150 A 20000612
OTHER SOURCE(S): MARPAT 136:37447
GI



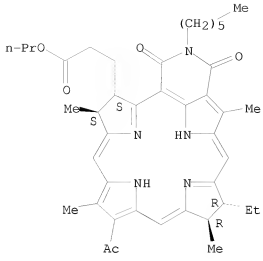
AB Novel compds. I [R1, R5, R9, R10 = independently C1-C3 alkyl (provided that at least 3 = Me); R2 = OH, OR11, NHR11, aryl or amino acid; R3, R4 = independently C(O)R11 or taken together = C(O)NR12C(O); R6, R7 = independently C1-C3; R8 = O-alkyl or S-alkyl, aryl or heterocyclic ring; R11 = C1-C6 alkyl; R12 = C1-C12 alkyl, aryl or aminoalkyl (C1-C8); provided that at least one of R8, R11, and R12 is hydrophobic and together contain at least 10 carbon atoms] that either preferentially absorb into hyperproliferative tissue and absorb light efficiently at a wavelength of between about 700 and about 850 nm or act as intermediates for such absorbing compds were prepared Thus, 3-deacetyl-3-(1-heptyloxyethyl)-bacteriopurpurin-N-hexylimide Pr ester (II) was prepared in 6 or 7 steps from bacteriochlorophyll A. The in vivo photosensitizing efficacy of II against a mouse tumor model system (RIF tumor) was evaluated. The invention also includes method of making and using the compds.

IT 182253-28-7P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(long wavelength absorbing bacteriochlorin alkyl ether analogs)

RN 182253-28-7 CAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:909501 CAPLUS <<LOGINID::20081001>>

DOCUMENT NUMBER: 136:179872

TITLE: Bacteriopurpurinimides: Highly Stable and Potent Photosensitizers for Photodynamic Therapy

AUTHOR(S): Chen, Yihui; Graham, Andrew; Potter, William; Morgan, Janet; Vaughan, Lurine; Bellnier, David A.; Henderson, Barbara W.; Oseroff, Allan; Dougherty, Thomas J.; Pandey, Ravindra K.

CORPORATE SOURCE: Photodynamic Therapy Center and Department of Dermatology, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA

SOURCE: Journal of Medicinal Chemistry (2002), 45(2), 255-258 CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The in situ conversion of the unstable bacteriochlorophyll a present in Rhodobacter sphaeroides produced highly stable bacteriopurpurin-18 which in a sequence of reactions was converted into a series of alkyl ether analogs of bacteriopurpurin-18-N-alkylimides with long wavelength absorption near 800 nm. The effective photosensitizers were found to localize in mitochondria but did not show any specific displacement of 3H-PK11195, suggesting that the mitochondrial peripheral benzodiazepine receptor is not the cellular binding site for this class of compds. The heptyl ether analog of bacteriopurpurin-18 showed excellent PDT efficacy in mice with implanted with fibrosarcoma cells.

IT 182253-28-7P

RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

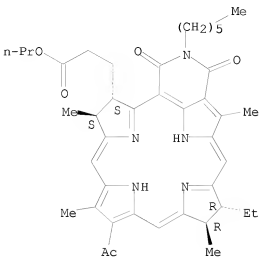
(preparation of and photosensitizing efficacy of bacteriopurpurin-18 analogs against fibrosarcoma)

RN 182253-28-7 CAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-19-hexyl-

1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:569737 CAPLUS <<LOGINID::20081001>>
DOCUMENT NUMBER: 125:275490
ORIGINAL REFERENCE NO.: 125:51513a,51516a
TITLE: Syntheses of stable bacteriochlorophyll-a derivatives as potential photosensitizers for photodynamic therapy
AUTHOR(S): Kozyrev, Andrei N.; Zheng, Gang; Zhu, Chunfeng; Dougherty, Thomas J.; Smith, Kevin M.; Pandey, Ravindra K.
CORPORATE SOURCE: Dep. Radiation Biol., Roswell Park Cancer Inst., Buffalo, NY, 14263, USA
SOURCE: Tetrahedron Letters (1996), 37(36), 6431-6434
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB New methods for conversion of unstable bacteriochlorophyll-a present in Rb. sphaeroides into stable bacteriochlorins are presented. Cyclic imide derivs. from related cyclic isoimide or amide analogs are obtained by intramol. base catalyzed cyclization. Most of the new bacteriochlorins have long wavelength absorptions in the range of 796-822 nm. In preliminary screening, the isoimide analogs have shown promising in vivo photosensitizing activity for the treatment of cancer by photodynamic therapy.

IT 182253-28-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(syntheses of stable bacteriochlorins as potential photosensitizers for photodynamic therapy)

RN 182253-28-7 CAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-19-hexyl-

1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (CA INDEX NAME)

Absolute stereochemistry.